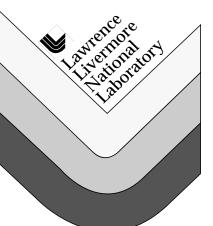
# SPATIALLY CONTINUOUS MIXED P<sub>2</sub>-P<sub>1</sub> SOLUTIONS FOR PLANAR GEOMETRY

Patrick S. Brantley

This paper was prepared for submittal to the ANS 2004 Winter Meeting November 14-18, 2004 Washington, D.C.

June 2004

This is a preprint of a paper intended for publication in a journal or proceedings. Since changes may be made before publication, this preprint is made available with the understanding that it will not be cited or reproduced without the permission of the author.



## DISCLAIMER

This document was prepared as an account of work sponsored by an agency of the United States Government. Neither the United States Government nor the University of California nor any of their employees, makes any warranty, express or implied, or assumes any legal liability or responsibility for the accuracy, completeness, or usefulness of any information, apparatus, product, or process disclosed, or represents that its use would not infringe privately owned rights. Reference herein to any specific commercial product, process, or service by trade name, trademark, manufacturer, or otherwise, does not necessarily constitute or imply its endorsement, recommendation, or favoring by the United States Government or the University of California. The views and opinions of authors expressed herein do not necessarily state or reflect those of the United States Government or the University of California, and shall not be used for advertising or product endorsement purposes

## Spatially Continuous Mixed P2-P1 Solutions for Planar Geometry

Patrick S. Brantley

Lawrence Livermore National Laboratory P.O. Box 808, L-023 Livermore, CA 94551 brantley1@llnl.gov

#### INTRODUCTION

Even-order Legendre polynomial (P<sub>N</sub>) expansion approximations of the neutron transport equation have historically seen only limited practical application. Research in the last decade [1] has resolved one of the historical theoretical objections [2] to the use of evenorder P<sub>N</sub> approximations in planar geometry, namely the ambiguity in the prescription of boundary conditions as a result of an odd number of unknowns. This research also demonstrated the P<sub>2</sub> approximation to be more accurate than the  $P_1$  approximation in planar geometry away from boundary layers and material interfaces. Neither the P<sub>1</sub> nor the P<sub>2</sub> approximation is convincingly more accurate near material interfaces. This progress motivated the reexamination of the multidimensional simplified P<sub>2</sub> (SP<sub>2</sub>) approximation [3], the development of  $P_2$  approximations for planar geometry stochastic transport problems [4], and the examination of the P<sub>2</sub> and SP<sub>2</sub> approximations as a synthetic acceleration technique for the discrete ordinates equations. [5]

The major remaining objection to even-order P<sub>N</sub> approximations is that the scalar flux distributions obtained using these approximations can exhibit large spatial discontinuities at material interfaces and source discontinuities. In contrast, the odd-order P<sub>N</sub> approximations typically utilized give spatially continuous scalar flux distributions at these locations. In this paper, we propose a mixed  $P_2$ - $P_1$  angular approximation designed to take advantage of the improved accuracy of the P<sub>2</sub> approximation in the interior of material regions and near external boundaries while retaining the continuous solutions obtained by the P<sub>1</sub> approximation near material interfaces and source discontinuities. We present numerical results from a series of eigenvalue calculations to demonstrate the accuracy of the mixed P<sub>2</sub>-P<sub>1</sub> angular approximation.

## THE MIXED P2-P1 ANGULAR APPROXIMATION

The P<sub>2</sub> angular approximation to the planar geometry neutron transport equation in a spatial domain  $0 \le x \le L$  can be written as [1]:

$$-\frac{d}{dx}\frac{1}{3\sigma_{a1}(x)}\frac{d}{dx}\hat{\phi}(x)+\hat{\sigma}_{a0}(x)\hat{\phi}(x)=\hat{Q}(x) \quad , \tag{1}$$

where

$$\hat{\sigma}_{a0}(x) = \frac{\sigma_{a0}(x)}{1 + \frac{4}{5}\rho(x)} \quad , \tag{2}$$

$$\hat{Q}(x) = \frac{Q(x)}{1 + \frac{4}{5}\rho(x)} \quad , \tag{3}$$

$$\hat{\phi}(x) = \left[1 + \frac{4}{5}\rho(x)\right]\phi_0(x) - \frac{4}{5}\rho(x)\frac{Q(x)}{\sigma_{a0}(x)} \quad , \tag{4}$$

and

$$\rho(x) = \frac{\sigma_{a0}(x)}{\sigma_{a2}(x)} \quad . \tag{5}$$

Here Q(x) is a neutron source,  $\sigma_{an}(x) = \sigma_t(x) - \sigma_{sn}(x)$ , n = 0, 1, 2, are the "absorption" cross sections obtained by subtracting the Legendre angular moments of the differential scattering cross section from the total cross section, and  $\phi_0(x)$  is the neutron scalar flux. Eq. (1) is a standard diffusion equation (with a modified absorption cross section and source) for the modified scalar flux unknown  $\hat{\phi}(x)$ . The neutron scalar flux,  $\phi_0(x)$ , is readily obtained from the unknown  $\hat{\phi}(x)$  using Eq. (4). Defining the parameter  $\rho(x)$  by Eq. (5) gives the P<sub>2</sub> approximation and setting  $\rho(x) = 0$  results in the standard P<sub>1</sub> approximation. Marshak vacuum boundary conditions for the P<sub>2</sub> approximation are given by [1]

$$\frac{1}{4} \left( \frac{1 + \frac{1}{2} \rho(x_b)}{1 + \frac{4}{5} \rho(x_b)} \right) \hat{\phi}(x_b) \mp \frac{1}{6\sigma_{a1}(x_b)} \frac{d}{dx} \hat{\phi}(x_b) = -\frac{3}{40} \frac{\rho(x_b)}{\sigma_{a0}(x_b)} \hat{Q}(x_b) , \begin{cases} x_b = 0 \\ x_b = L \end{cases}$$
(6)

In this paper, we propose to define the parameter  $\rho(x)$  by the equation

$$\rho(x) = \frac{\sigma_{a0}(x)}{\sigma_{a2}(x)} \left[ 1 - \exp(-p\sigma_t(x)d_i(x)) \right] , \qquad (7)$$

where p is a user-specified parameter and  $d_i(x)$  is the distance to the nearest material interface or source discontinuity at a given spatial point x. For p = 0, the pure  $P_1$  approximation is recovered for all x; for  $p \to \infty$ , the pure  $P_2$  approximation is obtained for all x. With this

representation for  $\rho(x)$  and  $1 \le p \ll \infty$  (e.g.  $p \approx 5$ ), the  $P_1$  approximation is used at material interfaces and source discontinuities and the angular approximation transitions smoothly to the  $P_2$  approximation within approximately one mean free path from the material interface or source discontinuity. The numerical solution of the mixed  $P_2$ - $P_1$  equations requires essentially the same computational expense as the solution of the standard  $P_1$  equations.

#### NUMERICAL RESULTS

In this section, we compare the accuracy of the mixed  $P_2$ - $P_1$  angular approximation to the pure  $P_1$  and  $P_2$  angular approximations for a series of two-region k-eigenvalue problems (numerical test problem IV.F of Ref. [1]). The test problem is a two-region, isotropically scattering critical slab 5.0 cm thick, with vacuum left and right boundaries and cross-section discontinuities at x=2.5 cm. The mathematical description of the transport problem is

$$\mu \frac{\partial}{\partial x} \psi(x, \mu) + \sigma_t \psi(x, \mu) = \frac{1}{2} \left[ \sigma_s(x) + \frac{\nu \sigma_f(x)}{k} \right]_{-1}^1 \psi(x, \mu') d\mu' , \quad 0 < x < 5 ,$$
(8a)

$$\psi(0,\mu) = 0 \quad , \quad 0 < \mu \le 1 \quad , \tag{8b}$$

$$\psi(5, \mu) = 0$$
 ,  $-1 \le \mu < 0$  . (8c)  
The material properties are  $\sigma_t = 1.0 \text{ cm}^{-1}$  across the two

regions of the slab,  $\sigma_s(x) = \sigma_s^l = variable$  in the left region,  $0 \le x < 2.5$  (see Table I), and  $\sigma_s(x) = \sigma_s^r = 0.99$  cm<sup>-1</sup> in the right region,  $2.5 < x \le 5$ . The fission cross section  $v\sigma_f(x)$  takes the values  $v\sigma_f^l = 0$  in the left region and  $v\sigma_f^r = v\sigma_f^{critical}$  in the right region of the slab. The critical values  $v\sigma_f^{critical}$  for each value of  $\sigma_s^l$  are

given in Table I (taken from Ref. [1]) and give  $S_{16}$  discrete ordinates transport values of k = 1.

The percent relative errors in the computed k eigenvalue obtained using the pure  $P_1$  and  $P_2$  angular approximations to Eqs. (8) are shown in Table I. The

approximations to Eqs. (8) are shown in Table I. The accuracy of both approximations degrades as  $\sigma_s^l$  decreases, i.e. as the left region becomes less diffusive and the magnitude of the material property discontinuity increases. However, the eigenvalues obtained using the  $P_2$  approximation are significantly more accurate than those obtained using the  $P_1$  approximation for all values of  $\sigma_s^l$ . The scalar flux distributions surrounding the material discontinuity are shown in Fig. 1. The  $P_1$  scalar flux is continuous at the material interface but is significantly in error both near the interface and away

from the interface. The  $P_2$  scalar flux is discontinuous at the material interface but is more accurate than the  $P_1$  solution away from the interface.

The transport problem was also solved using the mixed  $P_2$ - $P_1$  approximation with three values of the parameter p of Eq. (7), p = 2.5, 5, and 10. The scalar flux distributions near the material interface obtained using the mixed  $P_2$ - $P_1$  approximation are shown in Fig. 1. Larger values of p give scalar flux distributions with much of the character of the  $P_2$  solution except they are spatially continuous at the material interface. Smaller values of p give more diffusive scalar flux solutions. The percent relative errors for the k eigenvalues obtained

using the mixed  $P_2$ - $P_1$  approximation are shown in Table I. The mixed  $P_2$ - $P_1$  approximation is more accurate than the  $P_1$  approximation for all values of the parameter p and  $\sigma_s^l$  considered. For this test problem, smaller values of the parameter p give more accurate results for the k eigenvalue than larger values. With the exception of the  $\sigma_s^l = 0.99$  case, the mixed  $P_2$ - $P_1$  approximation is more accurate than both the  $P_1$  and the  $P_2$  approximations for all values of the parameter p.

#### CONCLUSIONS

In this paper, we showed that the  $P_2$  approximation could be modified to give spatially continuous scalar flux solutions at material interfaces and source discontinuities. The proposed modification uses the  $P_1$  angular approximation at material interfaces and source discontinuities and smoothly transitions to the  $P_2$  approximation within approximately a mean free path from the interface. Neither the  $P_1$  nor the  $P_2$  approximation is convincingly more accurate near material interfaces, so the  $P_1$  approximation can be utilized at these locations to give spatially continuous results. Numerical results from a series of k-eigenvalue test problems demonstrate that the mixed  $P_2$ - $P_1$  approximation can yield improvements in accuracy over both the pure  $P_1$  and  $P_2$  approximations employed alone.

### **ACKNOWLEDGMENTS**

This work was performed under the auspices of the U.S. Department of Energy by University of California, Lawrence Livermore National Laboratory under Contract W-7405-Eng-48.

## REFERENCES

1. R. P. Rulko, E. W. Larsen, "Variational Derivation and Numerical Analysis of P<sub>2</sub> Theory in Planar Geometry," *Nucl. Sci. Engr.*, **114**, 271 (1993).

- 2. B. Davison, *Neutron Transport Theory*, Oxford University Press, London (1957).
- 3. D. I. Tomašević, E. W. Larsen, "The Simplified P<sub>2</sub> Approximation," *Nucl. Sci. Engr.*, **122**, 309 (1996).
- 4. B. Su, G. C. Pomraning, "P<sub>1</sub>, P<sub>2</sub>, and Asymptotic Approximations for Stochastic Transport," *Nucl. Sci. Engr.*, **120**, 75 (1995).
- 5. T. Noh, W. F. Miller, Jr., "The Effectiveness of P<sub>2</sub> and Simplified P<sub>2</sub> Synthetic Accelerations in the Solutions of Discrete Ordinates Transport Equations," *Nucl. Sci. Engr.*, **124**, 18 (1996).

TABLE I. Percent Relative Errors in the Criticality Eigenvalue  $\,k\,$  .

				mixed P <sub>2</sub> -P <sub>1</sub>		
$\sigma_s^l$	$v\sigma_f^r = v\sigma_f^{critical}$	$\mathbf{P}_1$	$P_2$	p = 2.5	p = 5	p = 10
0.99	0.1408299	-8.54	+0.19	-1.66	-0.70	-0.23
0.90	0.1650953	-9.86	+1.58	-0.68	+0.50	+1.07
0.80	0.1803974	-11.13	+2.57	-0.20	+1.21	+1.90
0.70	0.1903208	-12.09	+3.29	+0.06	+1.65	+2.46
0.60	0.1974249	-12.84	+3.86	+0.21	+1.95	+2.87
0.50	0.2028380	-13.45	+4.34	+0.30	+2.16	+3.19
0.40	0.2071421	-13.96	+4.76	+0.35	+2.33	+3.44
0.30	0.2106719	-14.40	+5.12	+0.38	+2.46	+3.66
0.20	0.2136351	-14.79	+5.45	+0.39	+2.56	+3.84
0.15	0.2149489	-14.96	+5.60	+0.40	+2.61	+3.92

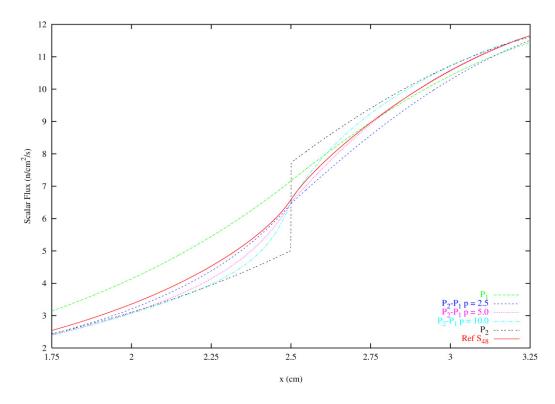


Fig. 1. Scalar flux near material property discontinuity for  $\sigma_s^l = 0.6$  case.

Technical Information Department · Lawrence Livermore National Laboratory University of California · Livermore, California 94551